

Do Topological Charge Solitons Participate in DNA Activity?

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We present a novel electromagnetic model of DNA molecules, in which the P-bonds act as tunnel junctions and the H-bonds as capacitors. Excess charge in the model gives rise to two coupled modified sine-Gordon equations, which admit topological solitonic excitations. We study the dynamics of the solitons, their effect on the DNA transport properties, and comment about their role in the DNA functioning. We propose specific experiments in order to test our predictions.

The DNA molecule is central to every living organism. It carries the genetic code of the organism, and continuously controls the synthesis of proteins, which are vital to its functioning and existence. Since the pioneering discoveries of Watson and Crick, a considerable effort was devoted to the study of the DNA, and much has been understood about its structure and activity [1]. Yet there are some key features which pose open questions. One such feature is the long range correlation and control between segments of the DNA. Synthesis of proteins is done via local "reading" of specific sectors in the DNA. The initiation of the reading is done by another segment, which can be located far away along the DNA sequence (thousands of bases away). Consider this and other examples [2], it seems as if the DNA molecule has the capability of transmitting information over long distances and in a specific manner (the information is transmitted to/from specific targets). Possible efficient candidates for such a transmission are solitons and solitary waves (rather than point particles/wave packets and linear waves). The existence and propagation of conformational solitons related to the DNA replication process have been studied in the past [3]. Non-topological charge solitons in proteins have also been studied [4]. Motivated by our studies of topological charge solitons in one dimensional (1D) arrays of mesoscopic tunnel junctions [5], [6], we have investigated the possibility of the existence of topological charge solitons in DNA.

We have developed a novel electromagnetical model of the DNA molecule, which is based on the properties of charge dynamics in the DNA (see Fig. 1). We view each of the DNA strands as a 1D array. A unit (or 'grain') of the array is a sugar and a base attached to it. The grains are connected longitudinally by Phosphate groups (P-bonds), and parallelly, i.e., to the other strand, by the Hydrogen bonds (H-bonds) between bases. An additional electron residing on an atom belonging to the sugar-base grain can hop from atom to atom, thus obtaining a kinetic energy. The H- and P-bonds form barriers to the charge propagation. The proton in the H-bond can effectively screen a net charge density on either side of the bond by shifting its position towards this side. (By 'net'

charge we mean the change from the charge distribution of the unperturbed DNA.) As a result, electrons do not cross the H-bond. Hence the bond can be viewed as a capacitor. The P-bond barrier stems from the two oxygens which are transversely connected to the phosphorus. These oxygens share three electrons with the phosphorus, giving rise to two σ bonds and one π bond. As the π electron can be shared with both oxygens, it behaves as an electron in a double well, and occupies the lowest level. When another electron approaches the well it encounters a barrier due to the energy difference to the next level of the well. However, since this barrier is narrow, the approaching electron can tunnel through the well. Thus from the charge dynamics point of view, the P-bond behaves as a tunnel junction.

We start with the model for a single strand (see Fig. 1). For simplicity we assume that all the bases are of the same type. Each grain i is composed of four sub-grains ($j = 0, 1, 2, 3$), assigned with phase variables, $\phi_{i,j}$. These phases are related to the electric potential of the sub-grains through $\phi_{i,j}(t) \equiv \frac{1}{\hbar} \int_{-\infty}^t V_{i,j}(t') dt'$. The conjugate variable to each $\phi_{i,j}$ is the charge on the sub-grain, $Q_{i,j}$. The Lagrangian of this model is

$$L = \sum_i \left[\frac{C}{2} (\dot{\phi}_{i+1,1} - \dot{\phi}_{i,3})^2 + \frac{C_S + C_0}{2} \dot{\phi}_{i,2}^2 + \frac{1}{2L/2} (\phi_{i,1} - \phi_{i,2})^2 - \frac{1}{2L/2} (\phi_{i,2} - \phi_{i,3})^2 + E_J \cos(\phi_{i+1,1} - \phi_{i,3}) - \frac{1}{L_0/2} (\phi_{i,0} - \phi_{i,2})^2 \right]. \quad (1)$$

It includes three types of energies: inductive energies which represent the hopping of electrons, capacitive energies which represent the capacitive properties of the H- and P-bonds, and a tunneling energy, which represents the tunneling process in the P-bond. This latter energy is proportional to the cosine of the phase difference across the bond, according to the tight binding picture [7]. The values of the parameters can be obtained, in principle, from experiments, but for now we employ only a qualitative view. The $L_0/2$ inductance denotes the hopping from the open side of a base to its sugar, while the $L/2$

inductance denotes the hopping between P-bonds. Since the former involves more hopping around carbon rings, we assume that $L_0 > L$. Both C_S and C_0 denote in this single-strand model capacitances to the outside world. C_S is the capacitance seen from the sugar, while C_0 is the capacitance seen from the open H-bond. We assume that both are of the same order of magnitude and much smaller than C , the capacitance of the P-bond tunnel junction. E_J is the tunneling strength of the P-bond. The length scale in our model, a , is the distance between grains, which is 3.4\AA . (In the model we use units in which $a = 1$.)

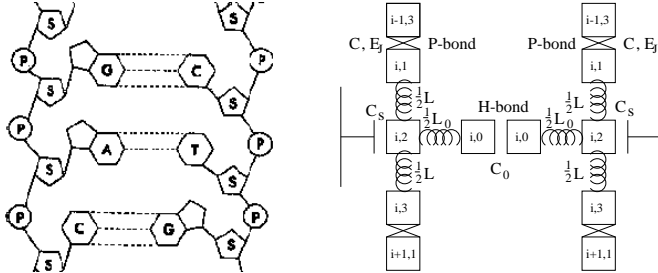


FIG. 1. A schematic image of a DNA molecule (left), and the double-strand model (right). On the left, P denote the P-bonds between the sugars S and the dashed lines are the H-bonds between the bases A,G,T and C. The parameters of the double-strand model are described in the text. In the single-strand case only one half of the model is used, and C_0 denotes the capacitance to the outside world.

From the kinetic part of (1) we see that out of the four variables describing the i 'th grain only three are independent. According to our experience in the study of 1D arrays of tunnel junctions [6], we introduce non-local (or integral) charge variables. These variables are very useful in trying to probe the collective, non-local dynamics of the DNA. We envision a propagation of charge from a certain point in the far left of the chain (' $-\infty$ ') to a certain point in the far right (' ∞ '), passing on its way the i 'th grain. Referring to the i 'th junction as the junction between the i 'th and the $(i+1)$ 'th grains, we define R_i as the charge that has *passed* through this junction:

$$R_i \equiv \sum_{i+1,1}^{\infty} Q_{i',j} = \sum_{i+1} (Q_{i',1} + Q_{i',2} + Q_{i',0} + Q_{i'}) - Q_{\infty} \\ = Q_{i,1} + \sum_{i+1} (Q_{i',2} + Q_{i',0}). \quad (2)$$

$\sum_{i+1,1}^{\infty} Q_{i',j}$ means summation over the sub-grain charges, starting from $(i' = i+1, j = 1)$ and going right, with the internal order $(i+1, 1) \rightarrow (i+1, 2) \rightarrow (i+1, 0) \rightarrow (i+1, 3) \rightarrow (i+2, 1)$, and so on. Next we define q_i as the charge that has *reached* junction i :

$$q_i \equiv \sum_{i,3}^{\infty} Q_{i',j} = Q_{i,3} + R_i = \sum_{i+1} (Q_{i',2} + Q_{i',0}). \quad (3)$$

After the canonical transformation to the variables: $\pi_i \equiv \phi_{i+1,2} - \phi_{i,2} - \theta_i$, $\theta_i \equiv \phi_{i+1,1} - \phi_{i,3}$ and $\dot{\phi}_{i,0} \equiv \dot{\phi}_{i,0} - \dot{\phi}_{i,2}$, we obtain the following Euclidean Lagrangian (in the continuum limit which we justify later):

$$L_E = \int dx \left\{ \frac{1}{2} L \dot{q}^2(x) - E_J \cos \theta(x) + \frac{1}{2} \frac{L_0}{2} \dot{q}_0^2(x) + \frac{1}{2C} [q(x) - R(x)]^2 + \frac{1}{2C_S} q_x^2(x) + \frac{1}{C_S} q_0(x) q_x(x) + \frac{1}{2C_{S0}} q_0^2(x) + i \dot{\theta}(x) R(x) \right\}, \quad (4)$$

where $C_{S0} \equiv C_S C_0 / (C_0 + C_S)$ is the effective capacitance across the chain (parallel coupling of C_S and C_0). As C_S is much smaller than C_0 , $C_{S0} \approx C_S$. We define a tunneling inductance $L_J \equiv \Phi_0^2 / (2\pi E_J)^2$ ($\Phi_0 \equiv h/e$ is the flux quantum), which we take to be much smaller than L . From (4) one can identify three characteristic frequencies in the system: $\Omega^2 \equiv 1/(LC)$ of the q mode, $\omega_J^2 \equiv 1/(L_J C)$ of the R mode, and $\omega^2 \equiv 2/(L_0 C_{S0})$ of the q_0 mode. In the limits we are working, we have $\Omega^2 \ll \omega_J^2, \omega^2$. Thus we can integrate out the R and q_0 modes, and obtain an effective theory for the q mode. The effective real time Lagrangian is

$$L^{eff} = \int dx \left\{ \frac{1}{2} L \dot{q}^2 - \frac{2}{(2\pi)^2} E_C \left[1 - \cos \left(\frac{2\pi}{e} q \right) \right] - \frac{1}{2(C_0 + C_S)} q_x^2 + \frac{1}{2} \frac{C_0^2 L_0}{2(C_0 + C_S)^2} \dot{q}_x^2 \right\}, \quad (5)$$

where $E_C \equiv e^2/(2C)$. The equation of motion of (5) is the following modified sine-Gordon equation:

$$L \ddot{q} + V_D \sin \left(\frac{2\pi}{e} q \right) - \frac{1}{C_0 + C_S} q_{xx} - \frac{C_0^2 L_0}{2(C_0 + C_S)^2} \ddot{q}_{xx} = 0, \quad (6)$$

where $V_D \equiv e/(2\pi C)$. This is a Kirchhoff law for the equivalent electrical circuit. Since the characteristic length scale in a sine-Gordon model is $C/(C_0 + C_S)$, the continuum limit is justified when $C > C_0 + C_S$, which indeed corresponds to our assumption. Transforming into dimensionless space, time and charge variables: $x \rightarrow x' \equiv \sqrt{C/C_0} x$, $t \rightarrow t' \equiv \sqrt{LC} t$, $q \rightarrow q' \equiv \frac{e}{2\pi} q$, we obtain:

$$\ddot{q} + \sin q - \frac{1}{1 + \mu_S} q_{xx} - \frac{\zeta}{2(1 + \mu_S)^2} \ddot{q}_{xx} = 0, \quad (7)$$

where $\zeta \equiv \frac{L_0 C_0}{LC}$, and $\mu_S \equiv C_S/C_0$.

Next we introduce the double-strand model (see again Fig. 1). We distinguish between the two strands by the superscripts α, β . The capacitance C_0 describes now the capacitive coupling between the two strands, i.e., over the H-bonds. We assume that it is much larger than the capacitance to the outside world, C_S , but still smaller than C . We take the parameters of the two strands to

be equal. Following the same steps of derivation as in the single-strand model (details will be given elsewhere [8]), we obtain two (dimensionless) coupled modified sine-Gordon equations of motion:

$$\ddot{\bar{q}} + \sin \bar{q} \cos q - \frac{1}{2\mu} \bar{q}_{xx} = 0, \quad (8)$$

$$\ddot{q} + \sin q \cos \bar{q} - \frac{1}{2(1+\mu)} q_{xx} - \frac{\zeta}{2(1+\mu)^2} \ddot{q}_{xx} = 0, \quad (9)$$

where $\mu \equiv C_S/2C_0$, and we have used the average and the relative charge variables:

$$\bar{q} \equiv \frac{1}{2} (q^\alpha + q^\beta) \quad q \equiv \frac{1}{2} (q^\alpha - q^\beta), \quad (10)$$

Similar equations, without the ζ term, were studied in the past in connection with the stacked Josephson junctions model [9].

We turn now to study the modified sine-Gordon equations we have derived, starting from the single-strand model. The pure Sine-Gordon equation has exact topological soliton solutions. We have checked numerically and found that the extra term in equation (7) does not effect the stability of the topological soliton solution, though it does induce interaction with the plasmons. This interaction causes the soliton to slowly radiate away its kinetic energy. Using the collective coordinate:

$$X = -\frac{1}{2\pi} \int q_x x dx, \quad (11)$$

we find that the soliton velocity actually oscillates with relatively high frequency, but its average is almost constant, decreasing only slightly over large period of time. Therefore, though the soliton's motion is not persistent in the exact sense, charge can propagate relatively large distances along the strand without the need to apply a driving force in the form of a potential difference.

The extra term in equation (7) destroys the Lorentz invariance of this equation. The dispersion relation for small amplitude linear waves is

$$\omega^2 = \frac{k^2/(1+\mu_S) + 1}{\frac{\zeta}{2}k^2/(1+\mu_S) + 1}, \quad (12)$$

and the group velocity tend to zero for both small and large k values. When the soliton velocity exceed the maximal group velocity, it leaves in its wake all the small amplitude waves.

In the double-strand model, the dimensionless parameter μ serves as a measure of the strength of the interaction between the strands (it is small for strong interaction). Since $C_S \ll C_0$, μ is very small. In the extreme $\mu = 0$ limit, \bar{q}_x should be zero as well, in order that the Lagrangian for this model would be finite. As both q^α and q^β have integer values at the two edges of the chain,

$\bar{q} \approx 2\pi n$ everywhere. We are thus left with a single equation for q :

$$\ddot{q} + \sin q - \frac{1}{2} q_{xx} - \frac{\zeta}{2} \ddot{q}_{xx} = 0. \quad (13)$$

This equation is equivalent to the one of the single-strand model, but now q represents a soliton anti-soliton pair (with zero total charge) rather than a single charged soliton.

Equations (8,9) have two simple topological solutions. One is the "symmetrical" solution, namely, $q = 0$ and \bar{q} is a usual Sine-Gordon kink. This solution is unstable, at least at low energy, since it corresponds to two charges with equal sign which tend to separate. It is, however, possible that it becomes stable at high energy, as was demonstrated for the stacked Josephson junctions model [10]. The other "anti-symmetrical" solution has $\bar{q} = 0$ and q in the form of a kink. It is a stable solution which correspond to an electron-hole pair (each on a different strand). It is plausible that this excitation is used in the DNA to transmit information over long distances. It can be created at a specific segment, which is responsible for the initiation of a certain protein synthesis, by tunneling of an electron through the H-bond (as a result of external agent). The pair can, then, propagate almost freely along the DNA, and be annihilated at the protein synthesis segment by a reverse tunneling, thus transmitting the order for this synthesis. The targeting of a specific annihilation segment is probably done through the specific base sequence of both segments, which was neglected in our model.

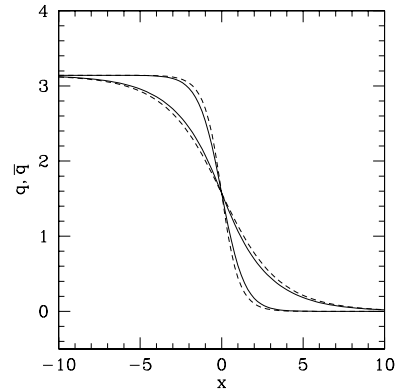


FIG. 2. Topological solution representing stationary charge in the α strand. The values $\mu = 0.1$ and $\zeta = 1$ were used. The steepest curve is $q(x)$, and the other is $\bar{q}(x)$. Numerical results are indicated by continuous lines and the theoretical curves of equation (14), by dashed lines.

There is also a way to approximate a solution which corresponds to an electron (hole) moving with velocity v in the, say, α strand:

$$\begin{aligned} q &= 2 \arctan \exp [-\gamma(x - vt)/c] \\ \bar{q} &= 2 \arctan \exp [-\bar{\gamma}(x - vt)/\bar{c}], \end{aligned} \quad (14)$$

where γ is the relativistic factor, and $c = 1/\sqrt{2(\mu+1)}$, $\bar{c} = 1/\sqrt{2\mu}$, are the linear wave velocities in equations (8,9) (when the last term in equation (9) is neglected). They correspond to the different linear waves velocity in the two equations. The exact solution can be obtained numerically and is shown in Fig. 2.

An important way to test our model is via measurements of the current-voltage characteristics. An electron can be injected to one of the strands to form a topological charge soliton, and may be subjected to an applied external voltage V and an Ohmic dissipation R (both per unit length). We implement this in our model by adding the terms $F + \alpha\dot{q}$ to equation (8) and $\alpha\dot{q}$ to equation (9), where $F \equiv V/V_D$ and $\alpha \equiv RC/\sqrt{LC}$, are the external force and the dissipation rate respectively. For given values of force and dissipation rate a soliton reaches a limiting velocity which corresponds to the measured current. The I-V curves which we obtain for different choices of the μ and ζ parameters are shown in Fig. 3. It should be noted that above some threshold voltage close to the maximum voltage indicated in each curve of Fig. 3, the system becomes unstable, as more and more soliton anti-soliton pairs are created.

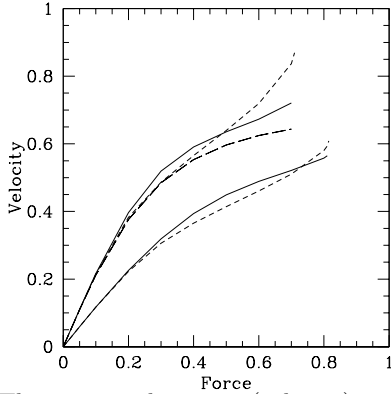


FIG. 3. The numerical current (velocity) - voltage (force) curves for a charge soliton propagating in one strand. In the lower curves $\alpha = 0.5$ and $\mu = 0.5$, while in the upper ones $\alpha = 0.5$ and $\mu = 0.05$. In the continuous lines $\zeta = 0.1$, and in the short dash lines $\zeta = 1$. The theoretical curve of equation (15) is indicated by a long dash line.

We proceed to estimate the limiting velocity. To do so, we equate the energy gain by the external force and the dissipative energy [11]. We find that $\dot{X}(\gamma/c + \bar{\gamma}/\bar{c}) = \pi F/2\alpha$. This reduces in the small μ limit to

$$\dot{X} = \frac{1}{\sqrt{2 \left[\left(\frac{2\alpha}{\pi F} \right)^2 + 1 \right]}}. \quad (15)$$

This theoretical curve is also shown in Fig. 3. The ascending of the numerical curve in the “relativistic” regime above the theoretical curve is obviously due to the ζ term.

We turn now to discuss some possible experimental tests of our predictions. The most straightforward test is to measure the I-V characteristics of a DNA that was mentioned earlier. Such experiments are now being developed [12]. We propose to use first a single strand vs a double strand. It is easier to inject solitons into the former. In the case of a double strand, it would be useful if each end is made of a short single strand (a different one on each end). In both cases it would be easier to compare the experimental results with the theoretical predictions if artificial strands composed of repetitions of one base are used. Another approach would be to study the magnetic response of circular strands. The idea is to place many circular strands on a surface, apply a time-dependent magnetic flux (say, of a saw tooth form), and measure the response of the system. For short circular strands at low temperature we expect to observe persistent current carried by the charge solitons. Finally, a less trivial experiment, is to inject a charge soliton at the end of the DNA via Scanning Tunneling Microscope (STM), and look for a response at the other end (for example, via an attached molecule that has a fluorescent response to an incoming charge).

These are just three examples of many more possible tests of our predictions about the existence of topological charge solitons in DNA molecules. If turned to be verified, we expect charge solitons to have crucial role in the DNA activities as means of transfer of information and energy over long distances, and to specific locations. To study this role, one can use our model as a starting point, incorporating into it the inhomogeneity of the chain due to the different bases, as well as interactions with external molecules at specific sites.

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